

1-Hexene  
592-41-6 | DTXSID4025402

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 296 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.82e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethylbenzene</div> <div>Measured: 170</div> <div>Predicted: 271</div>	<div>Image not found</div> <div>Styrene</div> <div>Measured: 912</div> <div>Predicted: 358</div>	<div>Image not found</div> <div>Toluene</div> <div>Measured: 117</div> <div>Predicted: 87.4</div>
<div>Image not found</div> <div>para-Xylene</div> <div>Measured: 257</div> <div>Predicted: 246</div>	<div>Image not found</div> <div>p-Cresol</div> <div>Measured: 501</div> <div>Predicted: 95.9</div>	